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Ultrafast dynamics of titanate octahedra tilting modes in a THz laser pulse MINGQIANG GU, JAMES M. RONDINELLI, Northwestern University — Using first-principles calculation, the electronic band structure and electric dipole moment for orthorhombic titanate are examined. To explore the energy dissipation after pulse excitation, the light-lattice coupling is treated with the mode oscillator model. By solving the equation of motion, we investigate the dynamics of the tilting modes. The evolution of the optical transition matrix elements as functions of different octahedra tilting modes and mode amplitudes are also evaluated, which provides theoretical base for the future experiments.

Mingqiang Gu
Northwestern University

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